Data Mining:

Concepts and Techniques

(3rd ed.)

— Chapter 10 —

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Chapter 10. Cluster Analysis: Basic Concepts and Methods

- Cluster Analysis: Basic Concepts
- Partitioning Methods
- Hierarchical Methods
- Density-Based Methods
- Grid-Based Methods
- Evaluation of Clustering
- Summary

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What is Cluster Analysis?

- Cluster: A collection of data objects
  - Similar (or related) to one another within the same group
  - Dissimilar (or unrelated) to the objects in other groups
- Cluster analysis (or *clustering*, *data segmentation, …*)
  - Finding similarities between data according to the characteristics found in the data and grouping similar data objects into clusters
- Unsupervised learning: NO predefined classes (i.e., learning by *observations* vs. learning by *examples*: supervised)
- Typical applications
  - As a stand-alone tool to get insight into data distribution
  - As a preprocessing step for other algorithms

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Clustering for Data Understanding and Applications

- Biology: taxonomy of living things: kingdom, phylum, class, order, family, genus and species （界.门.纲.目.科.属.种）
- Information retrieval: documer
- Land use: Identification of area observation database
- Marketing: Help marketers dis bases, and then use programs
- City-planning: Identify type, value, and geog
- Earth-quake studies: clustered along conti
- Climate: understandi and ocean movemen
- Economic Science: m

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Clustering as a Preprocessing Tool (Utility)

- Summarization:
  - Preprocessing for regression, PCA (why?), classification, and association analysis
- Compression:
  - Image processing: vector quantization
- **Finding K-nearest Neighbors**
  - *Localizing search* to one or a small number of clusters
- Outlier detection
  - Outliers are often viewed as those "far away" from any cluster

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Quality: What Is Good Clustering?

- A good clustering method will produce high quality clusters
  - high intra-class similarity: cohesive within clusters
  - low inter-class similarity: distinctive between clusters
- The quality of a clustering method depends on
  - the *similarity measure* used by the method
  - its implementation, and
  - Its ability to discover some or all of the hidden patterns

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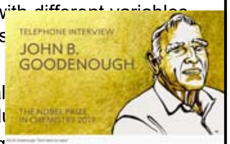
Measure the Quality of Clustering

- Dissimilarity/Similarity metric
  - Similarity is expressed in terms of a distance function, typically metric: *d(i, j)*
  - The definitions of distance functions are usually rather different for interval-scaled, boolean, categorical, ordinal ratio, and vector variables
  - **Weights** should be associated w
    based on applications and data s
- Quality of clustering:
  - There is usually a *separate* “qual
    measures the “goodness” of a cl
  - It is hard to define “similar enough” or “good enough”
    - The answer is typically highly subjective



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Considerations for Cluster Analysis

- Partitioning criteria
  - Single level vs. hierarchical partitioning (often, multi-level hierarchical partitioning is desirable)
- Separation of clusters
  - Exclusive (e.g., one customer belongs to only one region) vs. non-exclusive (e.g., one document may belong to more than one class) a.k.a. **multi-label** clustering (e.g., *community detection*)
- Similarity measure
  - **Distance**-based (e.g., Euclidian, road network, vector) vs. ***connectivity****-based* (e.g., density or contiguity)
- Clustering space
  - Full space (often when low dimensional) vs. *subspaces* (often in high-dimensional clustering)

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Requirements and Challenges

- **Scalability**
  - Clustering all the data instead of only on some samples
- Ability to deal with different types of attributes
  - Numerical, binary, categorical, ordinal, linked, and mixture of these
- **Constraint-based** clustering
  - User may give inputs on constraints
  - Use domain knowledge to determine input ***parameters***
- Interpretability and usability
- Others
  - Discovery of clusters with **arbitrary shapes** (e.g., Swiss swirl)
  - Ability to deal with noisy data
  - **Incremental clustering** and **insensitivity to input order**
  - High dimensionality

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Major Clustering Approaches (I)

- Partitioning approach:
  - Construct various partitions and then evaluate them by some criterion, e.g., minimizing the sum of square errors
  - Typical methods: k-means, k-medoids (PAM), CLARA
- Hierarchical approach:
  - Create a hierarchical decomposition of the set of data (or objects) using some criterion
  - Typical methods: Diana, Agnes, BIRCH, CAMELEON
- **Density-based approach**:
  - Based on connectivity and density functions
  - Typical methods: DBSACN, OPTICS, DenClue, *GraphCut*
- Grid-based approach:
  - Based on a multiple-level granularity structure
  - Typical methods: STING, WaveCluster, CLIQUE

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Major Clustering Approaches (II)

- Model-based:
  - A model is hypothesized for each of the clusters and tries to find the best fit of that model to each other
  - Typical methods: **EM**, SOM, COBWEB
- Frequent pattern-based:
  - Based on the analysis of frequent patterns
  - Typical methods: p-Cluster
- User-guided or **constraint-based**:
  - Clustering by considering user-specified or application-specific constraints
  - Typical methods: COD (obstacles), *constrained clustering*
- **Link-based** clustering:
  - Objects are often linked together in various ways
  - Massive links can be used to cluster objects: **SimRank, LinkClus**

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Partitioning Algorithms: Basic Concept

- Partitioning method: Partitioning a database ***D*** of ***n*** objects into a set of ***k*** clusters, such that the sum of squared distances is minimized (where c_i is the centroid or medoid of cluster C_i)

$$E = \Sigma_{i=1}^{k} \Sigma_{p \in C_i} (p - c_i)^2$$

- Given *k*, find a partition of *k clusters* that optimizes the chosen partitioning criterion
  - Global optimal: exhaustively enumerate all partitions
  - Heuristic methods: *k-means* and *k-medoids* algorithms
  - *k-means* (MacQueen'67, Lloyd'57/'82): Each cluster is represented by the center of the cluster
  - *k-medoids* or PAM (Partition Around Medoids) (Kaufman & Rousseeuw'87): Each cluster is represented by *one of the objects* in the cluster

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The *K-Means* Clustering Method

- Given *k*, the *k-means* algorithm is implemented in four steps:
  - Partition objects into *k* nonempty subsets
  - Compute seed points as the centroids of the clusters of the current partitioning (the centroid is the center, i.e., *mean point*, of the cluster)
  - Assign each object to the cluster with the nearest seed point
  - Go back to Step 2, stop when the assignment does not change

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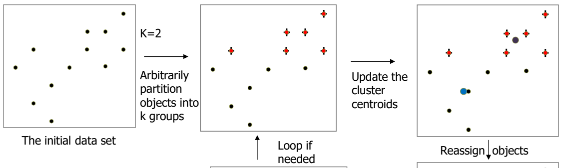
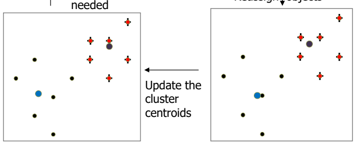
An Example of *K-Means* Clustering





- Partition objects into *k* nonempty subsets
- Repeat
  - Compute centroid (i.e., mean point) for each partition
  - Assign each object to the cluster of its nearest centroid
- Until no change

Alternatively, start with k arbitrary centroids

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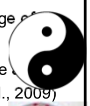
Comments on the *K-Means* Method

- Strength: *Efficient*: *O*(*tkn*), where *n* is # objects, *k* is # clusters, and *t* is # iterations. Normally, *k*, *t* << *n*.
    - Comparing: PAM: O(k(n-k)^2), CLARA: O(ks^2 + k(n-k))
- Comment: Often terminates at a *local optimum*. **(initialization can matter!)**
- Weakness
  - Applicable only to objects in a continuous n-dimensional space
    - Using the k-modes method for *categorical* data
    - In comparison, k-medoids can be applied to a *wider* range of data
  - Need to specify *k*, the *number* of clusters, **in advance** (there are ways to automatically determine the best k (see Hastie et al., 2009)
  - Sensitive to noisy data and *outliers*
  - Not suitable to discover clusters with ***non-convex shapes***



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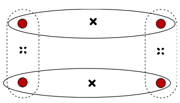
Variations of the *K-Means* Method

- Most of the variants of the *k-means* which **differ** in
  - Selection of the initial *k* means
  - Dissimilarity calculations
  - **Strategies to calculate cluster means**



- Handling categorical data: *k-modes*
  - Replacing means of clusters with modes (most popular value)
  - Using new dissimilarity measures to deal with categorical objects
  - Using a frequency-based method to update modes of clusters
  - A mixture of categorical and numerical data: *k-prototype* method

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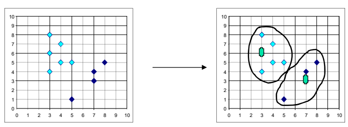
What Is the Problem of the K-Means Method?

- The k-means algorithm is sensitive to outliers !
  - Since an object with an extremely large value may substantially distort the distribution of the data (thus the mean calculation)
- K-Medoids: Instead of taking the **mean** value of the object in a cluster as a reference point, **medoids** can be used, which is the **most centrally located** object in a cluster



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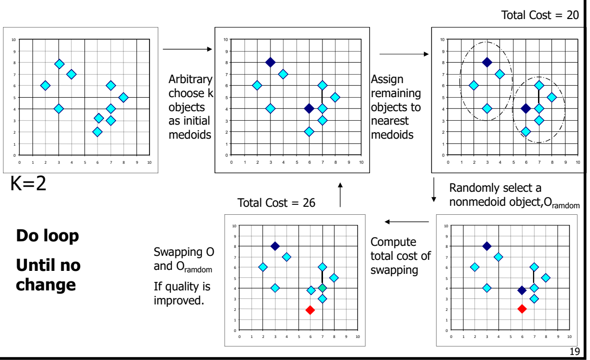
PAM: A Typical K-Medoids Algorithm



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The K-Medoid Clustering Method

- *K-Medoids* Clustering: Find *representative* objects (medoids) in clusters
  - *PAM* (Partitioning Around Medoids, Kaufmann & Rousseeuw 1987)
    - Starts from an initial set of medoids and iteratively replaces one of the medoids by one of the non-medoids if it improves the total distance of the resulting clustering
    - *PAM* works effectively for small data sets, but does not scale well for large data sets (due to the computational complexity)
- Efficiency improvement on PAM
  - *CLARA* (Kaufmann & Rousseeuw, 1990): PAM on *samples*
  - *CLARANS* (Ng & Han, 1994): *Randomized re-sampling*

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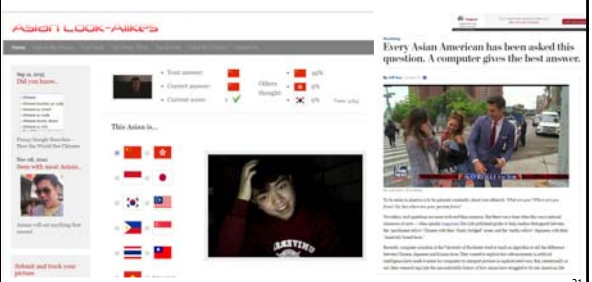
Do They All Look the Same?

- http://www.vista-today.com/asianmyth
- http://asianlookalikes.com/



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HW1-3 Graded before midterm

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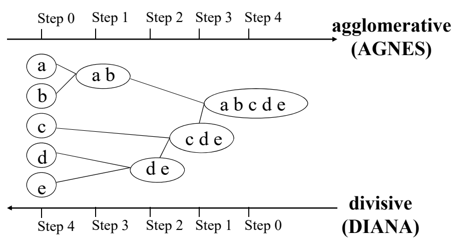
Hierarchical Clustering

- Use distance matrix as clustering criteria. This method does not require the number of clusters ***k*** as an input, but needs a termination condition



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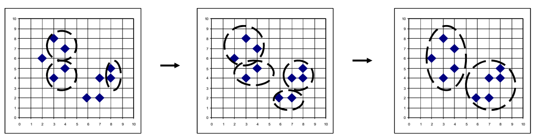
AGNES (Agglomerative Nesting)

- Introduced in Kaufmann and Rousseeuw (1990)
- Implemented in statistical packages, e.g., Splus
- Use the **single-link** method and the dissimilarity matrix
- Merge nodes that have the least dissimilarity
- Go on in a non-descending fashion
- Eventually all nodes belong to the same cluster



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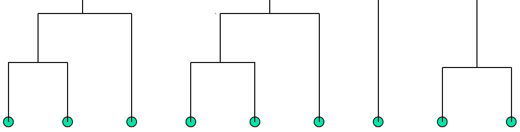
Dendrogram: Shows How Clusters are Merged

Decompose data objects into several levels of nested partitioning (tree of clusters), called a dendrogram

A clustering of the data objects is obtained by cutting the dendrogram at the desired level, then each connected component forms a cluster



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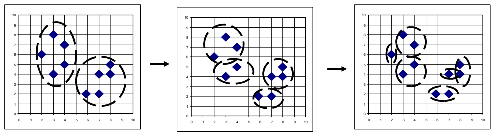
DIANA (Divisive Analysis)

- Introduced in Kaufmann and Rousseeuw (1990)
- Implemented in statistical analysis packages, e.g., Splus
- Inverse order of AGNES
- Eventually each node forms a cluster on its own



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Distance between Clusters

- Single link: smallest distance between an element in one cluster and an element in the other, i.e., $dist(K_i, K_j) = min(t_{ip}, t_{jq})$
- Complete link: largest distance between an element in one cluster and an element in the other, i.e., $dist(K_i, K_j) = max(t_{ip}, t_{jq})$
- Average: avg distance between an element in one cluster and an element in the other, i.e., $dist(K_i, K_j) = avg(t_{ip}, t_{jq})$
- Centroid: distance between the centroids of two clusters, i.e., $dist(K_i, K_j) = dist(C_i, C_j)$
- Medoid: distance between the medoids of two clusters, i.e., $dist(K_i, K_j) = dist(M_i, M_j)$
  - Medoid: a chosen, centrally located object in the cluster

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Centroid, Radius and Diameter of a Cluster (for numerical data sets)

- Centroid: the "middle" of a cluster

$$C_m = \frac{\Sigma_{i=1}^{N}(t_{ip})}{N}$$

- Radius: square root of average distance from any point of the cluster to its **centroid**

$$R_m = \sqrt{\frac{\Sigma_{i=1}^{N}(t_{ip}-c_m)^2}{N}}$$

- **Diameter**: square root of average mean squared distance between all **pairs** of points in the cluster

$$D_m = \sqrt{\frac{\Sigma_{i=1}^{N}\Sigma_{i=1}^{N}(t_{ip}-t_{iq})^2}{N(N-1)}}$$

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Extensions to Hierarchical Clustering

- Major weakness of agglomerative clustering methods
  - Can never undo what was done previously
  - Do not scale well: time complexity of at least $O(n^2)$, where n is the number of total objects
- Integration of hierarchical & distance-based clustering
  - BIRCH (1996): uses CF-tree and incrementally adjusts the quality of sub-clusters
  - CHAMELEON (1999): hierarchical clustering using dynamic modeling

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BIRCH (Balanced Iterative Reducing and Clustering Using Hierarchies)

SKIP>>

- Zhang, Ramakrishnan & Livny, SIGMOD'96
- Incrementally construct a CF (Clustering Feature) tree, a hierarchical data structure for multiphase clustering
  - Phase 1: scan DB to build an initial in-memory CF tree (a multi-level compression of the data that tries to preserve the inherent clustering structure of the data)
  - Phase 2: use an ***arbitrary*** clustering algorithm to cluster the leaf nodes of the CF-tree
- *Scales linearly*: finds a good clustering with a single scan and improves the quality with a few additional scans
- *Weakness:* handles only numeric data, and sensitive to the *order* of the data record

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Clustering Feature Vector in BIRCH

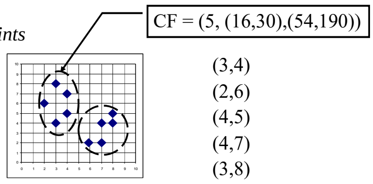
Clustering Feature (CF): ***CF = (N, LS, SS)***

N: **Number of data points**

LS: linear sum of N points: $\sum_{i=1}^{N} X_i$

SS: square sum of N points

$\sum_{i=1}^{N} X_i^2$



(3,4)
(2,6)
(4,5)
(4,7)
(3,8)

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CF-Tree in BIRCH

- Clustering feature:
  - Summary of the statistics for a given subcluster: the 0-th, 1st, and 2nd moments of the subcluster from the statistical point of view
  - Registers crucial measurements for computing cluster and utilizes storage efficiently
- A CF tree is a height-balanced tree that stores the clustering features for a hierarchical clustering
  - A nonleaf node in a tree has descendants or "children"
  - The nonleaf nodes store **sums** of the CFs of their children
- A CF tree has two parameters
  - Branching factor: max # of children
  - Threshold: *max diameter* of sub-clusters stored at the leaf nodes

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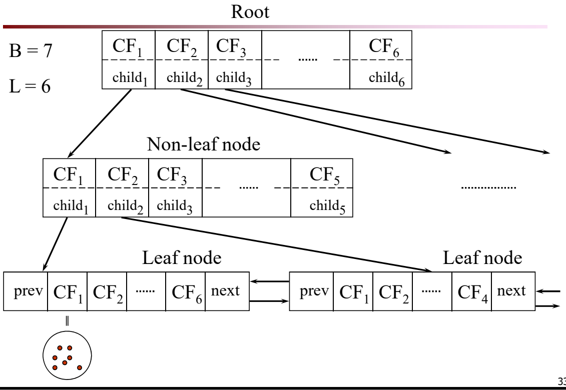
The CF Tree Structure



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The Birch Algorithm

- Cluster Diameter $\sqrt{\frac{1}{n(n-1)}\sum (x_i - x_j)^2}$
- For each point in the input
  - Find closest leaf entry
  - Add point to leaf entry and update CF
  - If entry diameter > max_diameter, then split leaf, and possibly parents
- Algorithm is O(n)
- Concerns
  - Sensitive to *insertion order* of data points
  - Since we *fix the size* of leaf nodes, so clusters may not be so natural
  - Clusters tend to be *spherical* given the radius and diameter measures

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CHAMELEON: Hierarchical Clustering Using Dynamic Modeling (1999)

- CHAMELEON: G. Karypis, E. H. Han, and V. Kumar, 1999
- Measures the similarity based on a *dynamic* model
  - Two clusters are merged only if the *interconnectivity* and *closeness (proximity)* between two clusters are high *relative to* the internal interconnectivity of the clusters and closeness of items within the clusters
- **Graph-based**, and a two-phase algorithm
  1. Use a graph-partitioning algorithm: cluster objects into a large number of relatively small sub-clusters
  2. Use an agglomerative hierarchical clustering algorithm: find the genuine clusters by repeatedly combining these sub-clusters

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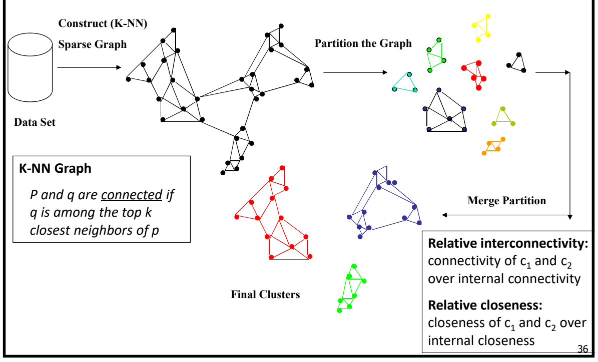
Overall Framework of CHAMELEON



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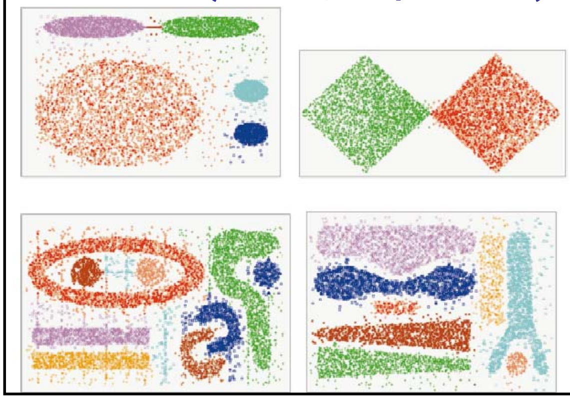
CHAMELEON (Clustering Complex Objects)



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Probabilistic Hierarchical Clustering

- *Algorithmic* hierarchical clustering
  - Nontrivial to choose a good distance measure
  - Hard to handle missing attribute values
  - Optimization goal not clear: *heuristic, local search*
- *Probabilistic* hierarchical clustering
  - Use probabilistic models to measure distances between clusters
  - Generative model: Regard the set of data objects to be clustered as a sample of the underlying data generation mechanism to be analyzed
  - Easy to understand, same efficiency as algorithmic agglomerative clustering method, can handle partially observed data
- In practice, assume the generative models adopt common distributions functions, e.g., Gaussian distribution or Bernoulli distribution, governed by parameters

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Generative Model

- Given a set of 1-D points $X = \{x_1, \ldots, x_n\}$ for clustering analysis & assuming they are generated by a Gaussian distribution:

$$\mathcal{N}(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

- The probability that a point $x_i \in X$ is generated by the model

$$P(x_i|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- The likelihood that X is generated by the model:

i.i.d.

$$L(\mathcal{N}(\mu, \sigma^2) : X) = P(X|\mu, \sigma^2) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- The task of learning the generative model: find the parameters μ and σ^2 such that

the maximum likelihood

$$\mathcal{N}(\mu_0, \sigma_0^2) = \arg\max\{L(\mathcal{N}(\mu, \sigma^2) : X)\}$$

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A Probabilistic Hierarchical Clustering Algorithm

- For a set of objects partitioned into m clusters $C_1, \ldots, C_m$, the quality can be measured by,

$$Q(\{C_1, \ldots, C_m\}) = \prod_{i=1}^{m} P(C_i)$$

  where $P()$ is the maximum likelihood
- **Distance** between clusters C_1 and C_2: $dist(C_i, C_j) = -\log \frac{P(C_1 \cup C_2)}{P(C_1)P(C_2)}$
- Algorithm: Progressively merge points and clusters
  - Input: $D = \{o_1, \ldots, o_n\}$: a data set containing n objects
  - Output: A hierarchy of clusters
  - Method
    - Create a cluster for *each* object $C_i = \{o_i\}$, $1 \le i \le n$;
    - For i = 1 to n {
      - Find pair of clusters C_i and C_j such that
        - $C_i, C_j = \text{argmax}_{i \neq j} \{\log (P(C_i \cup C_j)/(P(C_i)P(C_j)))\}$;
      - If $\log (P(C_i \cup C_j)/(P(C_i)P(C_j))) > 0$ then merge C_i and C_j }

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Density-Based Clustering Methods

- Clustering based on density (local cluster criterion), such as *density-connected* points
- Major features:
  - Discover clusters of *arbitrary shape*
  - Handle noise
  - One scan
  - Need density parameters as termination condition
- Several interesting studies:
  - DBSCAN: Ester, et al. (KDD'96)
  - OPTICS: Ankerst, et al (SIGMOD'99).
  - DENCLUE: Hinneburg & D. Keim (KDD'98)
  - CLIQUE: Agrawal, et al. (SIGMOD'98) (more grid-based)

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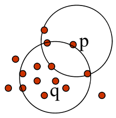
Density-Based Clustering: Basic Concepts

- Two parameters:
  - *Eps*: Maximum radius of the neighbourhood
  - *MinPts*: Minimum number of points in an Eps-neighbourhood of that point
- $N_{Eps}(p)$: {q belongs to D | dist(p,q) ≤ Eps}
- Directly density-reachable: A point *p* is directly *density-reachable* from a point *q* w.r.t. *Eps*, *MinPts* if
  - *p* belongs to $N_{Eps}(q)$
  - ***core*** point condition:

    $|N_{Eps}(q)| \geq MinPts$

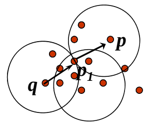


MinPts = 5

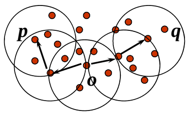
Eps = 1 cm

Density-Reachable and Density-Connected

- Density-reachable:
  - A point *p* is density-reachable from a point *q* w.r.t. *Eps*, *MinPts* if there is a chain of points $p_1, \ldots, p_n$, $p_1 = q$, $p_n = p$ such that p_{i+1} is directly density-reachable from p_i

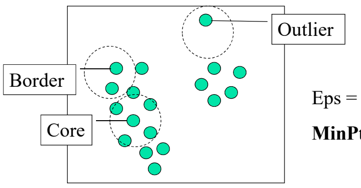


- Density-connected
  - A point *p* is density-connected to a point *q* w.r.t. *Eps*, *MinPts* if there is a point *o* such that both, *p* and *q* are density-reachable from *o* w.r.t. *Eps* and *MinPts*



DBSCAN: Density-Based Spatial Clustering of Applications with Noise

- Relies on a *density-based* notion of cluster: A *cluster* is defined as a maximal set of density-connected points
- Discovers clusters of arbitrary shape in spatial databases with noise



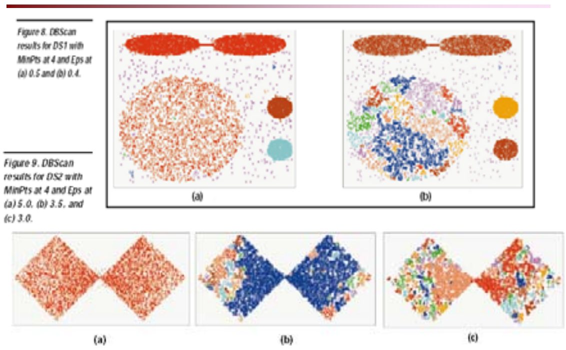
Eps = 1cm

MinPts = 5

DBSCAN: The Algorithm

- Arbitrary select a point *p*
- Retrieve all points (directly*) density-reachable from *p* w.r.t. *Eps* and *MinPts*
- If *p* is a core point, a cluster is formed
- If *p* is a border point*, (or) no points are density-reachable from *p* and DBSCAN visits the next point of the database
- Continue the process until all of the points have been processed

DBSCAN: Sensitive to Parameters

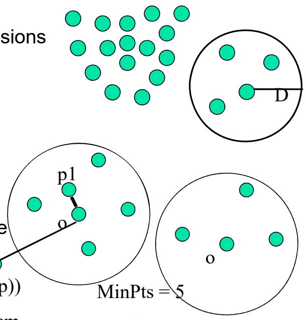


OPTICS: A Cluster-Ordering Method (1999)

- OPTICS: Ordering Points To Identify the Clustering Structure
  - Ankerst, Breunig, Kriegel, and Sander (SIGMOD'99)
  - Produces a special order of the database wrt its density-based clustering structure
  - This cluster-ordering contains info equiv. to the density-based clusterings corresponding *to a broad range of parameter settings (s.t. insensitive to parameters)*
  - Good for *both automatic and interactive* cluster analysis, including finding intrinsic clustering structure
  - Can be represented graphically or using visualization techniques

OPTICS: Some Extension from DBSCAN

- Index-based:
  - k = number of dimensions
  - N = 20
  - p = 75%
  - M = N(1-p) = 5
  - Complexity: O(*NlogN*)
- Core Distance:
  - min eps s.t. point is core
- Reachability Distance



Max (core-distance (o), d (o, p))

r(p1, o) = 2.8cm. r(p2,o) = 4cm

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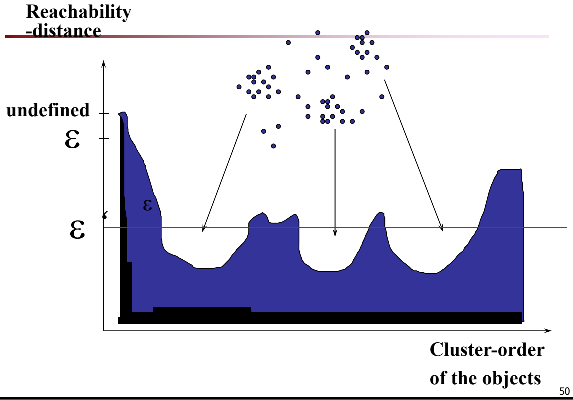

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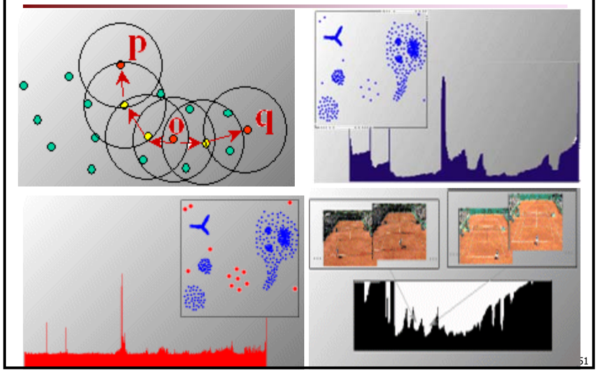
Density-Based Clustering: OPTICS & Its Applications



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DENCLUE: Using Statistical Density Functions

- DENsity-based CLUstEring by Hinneburg & Keim (KDD'98)
- Using statistical density functions:

$$f_{Gaussian}(x,y) = e^{-\frac{d(x,y)^2}{2\sigma^2}}$$

influence of y on x

$$f^D_{Gaussian}(x) = \sum_{i=1}^{N} e^{-\frac{d(x,x_i)^2}{2\sigma^2}}$$

total influence on x

$$\nabla f^D_{Gaussian}(x,x_i) = \sum_{i=1}^{N} (x_i - x)\cdot e^{-\frac{d(x,x_i)^2}{2\sigma^2}}$$

gradient of x in the direction of x_i

- Major features
  - Solid mathematical foundation
  - Good for data sets with large amounts of noise
  - Allows a compact mathematical description of arbitrarily shaped clusters in high-dimensional data sets (i.e., mixture of Gaussian)
  - Significantly faster than existing algorithm (e.g., DBSCAN)
  - But needs a large number of parameters

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Denclue: Technical Essence

- Uses grid cells but only keeps information about grid cells that do *actually* contain data points and manages these cells in a tree-based access structure
- Influence function: describes the impact of a data point within its neighborhood
- Overall density of the data space can be calculated as the sum of the influence function of all data points
- Clusters can be determined mathematically by identifying density attractors
- Density attractors are local maximal of the overall density function
- Center defined clusters: assign to each density attractor the points density attracted to it
- Arbitrary shaped cluster: merge density attractors that are connected through paths of high density (> threshold)

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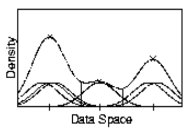
Density Attractor

(a) Data Set

(c) Gaussian



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Center-Defined and Arbitrary

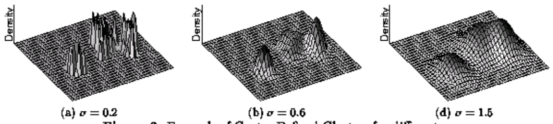

Figure 3: Example of Center-Defined Clusters for different σ

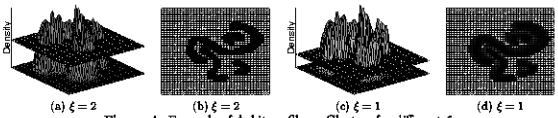

Figure 4: Example of Arbitray-Shape Clusters for different ξ

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Chapter 10. Cluster Analysis: Basic Concepts and Methods

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Grid-Based Clustering Method

- Using multi-resolution grid data structure
- Several interesting methods
  - STING (a STatistical INformation Grid approach) by Wang, Yang and Muntz (1997)
  - WaveCluster by Sheikholeslami, Chatterjee, and Zhang (VLDB'98)
    - A *multi-resolution* clustering approach using *wavelet* method
  - CLIQUE: Agrawal, et al. (SIGMOD'98)
    - Both grid-based and subspace clustering

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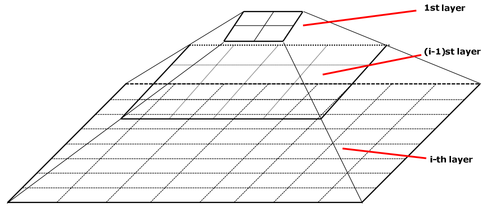
STING: A Statistical Information Grid Approach

- Wang, Yang and Muntz (VLDB'97)
- The spatial area is divided into rectangular cells
- There are several *levels* of cells corresponding to different levels of resolution



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The STING Clustering Method

- Each cell at a high level is partitioned into a number of smaller cells in the next lower level
- Statistical info of each cell is calculated and stored beforehand and is used to answer queries
- Parameters of higher level cells can be easily calculated from parameters of lower level cell
  - *count*, *mean*, *s*, *min*, *max*
  - type of distribution—*normal*, *uniform*, etc.
- Use a top-down approach to answer spatial data queries
- Start from a pre-selected layer—typically with a small number of cells
- For each cell in the current level compute the confidence interval

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STING Algorithm and Its Analysis

- Remove the irrelevant cells from further consideration
- When finish examining the current layer, proceed to the next lower level
- Repeat this process until the bottom layer is reached
- Advantages:
  - Query-independent, easy to parallelize, incremental update
  - *O(K)*, where *K* is the number of grid cells at the lowest level
- Disadvantages:
  - All the cluster boundaries are either horizontal or vertical, and no diagonal boundary is detected

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CLIQUE (Clustering In QUEst)

- Agrawal, Gehrke, Gunopulos, Raghavan (SIGMOD'98)
- Automatically identifying subspaces of a high dimensional data space that allow better clustering than original space
- CLIQUE can be considered as both density-based and grid-based
  - It partitions each dimension into the same number of equal length interval
  - It partitions an m-dimensional data space into non-overlapping rectangular units
  - A unit is dense if the fraction of total data points contained in the unit exceeds the input model parameter
  - A cluster is a maximal set of connected dense units within a subspace

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CLIQUE: The Major Steps

- Partition the data space and find the number of points that lie inside each cell of the partition.
- Identify the *subspaces* that contain clusters using the Apriori principle
- Identify clusters
  - Determine dense units in all subspaces of interests
  - Determine connected dense units in all subspaces of interests.
- Generate minimal description for the clusters
  - Determine maximal regions that cover a cluster of *connected* dense units for each cluster
  - Determination of minimal cover for each cluster

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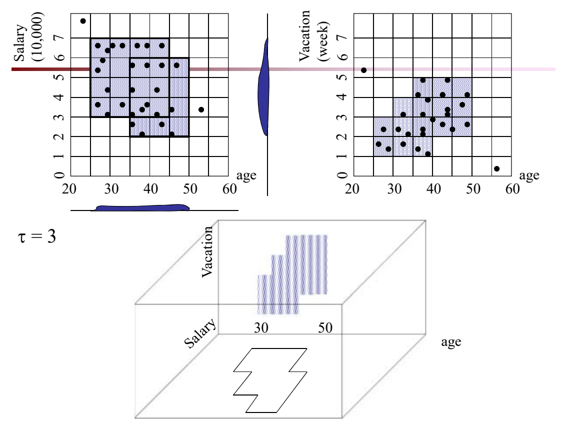

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Strength and Weakness of *CLIQUE*

- Strength
  - *automatically* finds subspaces of the highest dimensionality such that high density clusters exist in those subspaces
  - *insensitive* to the order of records in input and does not presume some canonical data distribution
  - scales *linearly* with the size of input and has good scalability as the number of dimensions in the data increases
- Weakness
  - The accuracy of the clustering result may be degraded at the expense of simplicity of the method

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Assessing Clustering Tendency

- Assess if non-random structure exists in the data by measuring the probability that the data is generated by a *uniform* data distribution
- Test spatial randomness by statistic test: Hopkins Static
  - Given a dataset D regarded as a sample of a random variable o, determine *how far away* o is from being uniformly distributed in the data space
  - Sample *n* points, $p_1, \ldots, p_n$, uniformly from D. For each p_i, find its nearest neighbor in D: $x_i = min\{dist(p_i, v)\}$ where *v* in D
  - Sample *n* points, $q_1, \ldots, q_n$, uniformly from D. For each q_i, find its nearest neighbor in D – $\{q_i\}$: $y_i = min\{dist(q_i, v)\}$ where *v* in D and $v \neq q_i$
  - Calculate the Hopkins Statistic: $H = \frac{\sum_{i=1}^{n} y_i}{\sum_{i=1}^{n} x_i + \sum_{i=1}^{n} y_i}$

  - If D is uniformly distributed, $\sum x_i$ and $\sum y_i$ will be close to each other and H is close to 0.5. If D is highly skewed, H is close to 0

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Determine the Number of Clusters

- Empirical method
  - # of clusters ≈ $\sqrt{n/2}$ for a dataset of n points
- Elbow method
  - Use the turning point in the curve of sum of within cluster variance w.r.t the # of clusters
- **Cross validation** method
  - Divide a given data set into *m* parts
  - Use *m* – 1 parts to obtain a clustering model
  - Use the remaining part to test the quality of the clustering
    - E.g., For each point in the test set, find the closest centroid, and use the sum of squared distance between all points in the test set and the closest centroids to measure how well the model fits the test set
  - For any k > 0, repeat it *m* times, compare the overall quality measure w.r.t. different *k*'s, and find # of clusters that fits the data the best

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Measuring Clustering Quality

- Two methods: extrinsic vs. intrinsic
- Extrinsic: supervised, i.e., the ground truth is *available*
  - Compare a clustering against the ground truth using certain clustering quality measure
  - Ex. BCubed *precision* and *recall* metrics
- Intrinsic: unsupervised, i.e., the ground truth is *unavailable*
  - Evaluate the goodness of a clustering by considering how well the clusters are separated, and how compact the clusters are
  - Ex. Silhouette coefficient, BIC (Bayesian Information Criterion), AIC (Akaike information criterion)

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Measuring Clustering Quality: Extrinsic Methods

- Clustering quality measure: $Q(C, C_g)$, for a clustering C given the ground truth C_g.
- Q is good if it satisfies the following **4** essential criteria
  - Cluster *homogeneity*: the purer, the better
  - Cluster *completeness*: should assign objects belong to the same category in the ground truth to the same cluster
  - Rag bag: putting a heterogeneous object into a pure cluster should be penalized more than putting it into a *rag bag* (i.e., "miscellaneous" or "other" category)
  - Small cluster preservation: splitting a small category into pieces is more harmful than splitting a large category into pieces

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Summary

- Cluster analysis groups objects based on their similarity and has wide applications
- Measure of similarity can be computed for various types of data
- Clustering algorithms can be categorized into partitioning methods, hierarchical methods, density-based methods, grid-based methods, and model-based methods
- K-means and K-medoids algorithms are popular partitioning-based clustering algorithms
- Birch and Chameleon are interesting hierarchical clustering algorithms, and there are also probabilistic hierarchical clustering algorithms
- DBSCAN, OPTICS, and DENCLU are interesting density-based algorithms
- STING and CLIQUE are grid-based methods, where CLIQUE is also a subspace clustering algorithm
- Quality of clustering results can be evaluated in various ways

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Homework Assignment #5

- Textbook
  - 10.2, 10.4, 10.6
  - **More** after the midterm review
  - May include using some toolboxes

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References (1)

- R. Agrawal, J. Gehrke, D. Gunopulos, and P. Raghavan. Automatic subspace clustering of high dimensional data for data mining applications. SIGMOD'98
- M. R. Anderberg. Cluster Analysis for Applications. Academic Press, 1973.
- M. Ankerst, M. Breunig, H.-P. Kriegel, and J. Sander. Optics: Ordering points to identify the clustering structure, SIGMOD'99.
- Beil F., Ester M., Xu X.: "Frequent Term-Based Text Clustering", KDD'02
- M. M. Breunig, H.-P. Kriegel, R. Ng, J. Sander. LOF: Identifying Density-Based Local Outliers. SIGMOD 2000.
- M. Ester, H.-P. Kriegel, J. Sander, and X. Xu. A density-based algorithm for discovering clusters in large spatial databases. KDD'96.
- M. Ester, H.-P. Kriegel, and X. Xu. Knowledge discovery in large spatial databases: Focusing techniques for efficient class identification. SSD'95.
- D. Fisher. Knowledge acquisition via incremental conceptual clustering. Machine Learning, 2:139-172, 1987.
- D. Gibson, J. Kleinberg, and P. Raghavan. Clustering categorical data: An approach based on dynamic systems. VLDB'98.
- V. Ganti, J. Gehrke, R. Ramakrishan. CACTUS Clustering Categorical Data Using Summaries. KDD'99.

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References (2)

- D. Gibson, J. Kleinberg, and P. Raghavan. Clustering categorical data: An approach based on dynamic systems. In Proc. VLDB'98.
- S. Guha, R. Rastogi, and K. Shim. Cure: An efficient clustering algorithm for large databases. SIGMOD'98.
- S. Guha, R. Rastogi, and K. Shim. ROCK: A robust clustering algorithm for categorical attributes. In *ICDE'99*, pp. 512-521, Sydney, Australia, March 1999.
- A. Hinneburg, D.l A. Keim: An Efficient Approach to Clustering in Large Multimedia Databases with Noise. KDD'98.
- A. K. Jain and R. C. Dubes. Algorithms for Clustering Data. Printice Hall, 1988.
- G. Karypis, E.-H. Han, and V. Kumar. CHAMELEON: A Hierarchical Clustering Algorithm Using Dynamic Modeling. *COMPUTER*, 32(8): 68-75, 1999.
- L. Kaufman and P. J. Rousseeuw. Finding Groups in Data: an Introduction to Cluster Analysis. John Wiley & Sons, 1990.
- E. Knorr and R. Ng. Algorithms for mining distance-based outliers in large datasets. VLDB'98.

75

75

References (3)

- G. J. McLachlan and K.E. Bkasford. Mixture Models: Inference and Applications to Clustering. John Wiley and Sons, 1988.
- R. Ng and J. Han. Efficient and effective clustering method for spatial data mining. VLDB'94.
- L. Parsons, E. Haque and H. Liu, Subspace Clustering for High Dimensional Data: A Review, SIGKDD Explorations, 6(1), June 2004
- E. Schikuta. Grid clustering: An efficient hierarchical clustering method for very large data sets. Proc. 1996 Int. Conf. on Pattern Recognition
- G. Sheikholeslami, S. Chatterjee, and A. Zhang. WaveCluster: A multi-resolution clustering approach for very large spatial databases. VLDB'98.
- A. K. H. Tung, J. Han, L. V. S. Lakshmanan, and R. T. Ng. Constraint-Based Clustering in Large Databases, ICDT'01.
- A. K. H. Tung, J. Hou, and J. Han. Spatial Clustering in the Presence of Obstacles, ICDE'01
- H. Wang, W. Wang, J. Yang, and P.S. Yu. Clustering by pattern similarity in large data sets, SIGMOD'02
- W. Wang, Yang, R. Muntz, STING: A Statistical Information grid Approach to Spatial Data Mining, VLDB'97
- T. Zhang, R. Ramakrishnan, and M. Livny. BIRCH : An efficient data clustering method for very large databases. SIGMOD'96
- X. Yin, J. Han, and P. S. Yu, “LinkClus: Efficient Clustering via Heterogeneous Semantic Links”, VLDB'06

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